Results in Physics 6 (2016) 258–262

Contents lists available at ScienceDirect

Results in Physics

journal homepage: www.journals.elsevier.com/results-in-physics

Nonlocal heat transfer in two-dimensional Lennard–Jones crystal: Application of the molecular dynamics method

M.N. Ovchinnikov *, G.G. Kushtanova

Physics Department, Kazan Federal University, Russia

ARTICLE INFO

Article history:
Received 14 January 2016
Accepted 14 May 2016
Available online 20 May 2016

Keywords:
Molecular dynamics
Heat flux
Relaxation time
Lennard–Jones potential
Nonlinear telegrapher equation
The finite velocity of perturbations propagation

ABSTRACT

The redistribution of heat between two subsystems in the two-dimensional crystal consisting of particles interacting by means of the Lennard–Jones potential with argon parameters is considered in the frame of molecular dynamics method. Calculations of heat flux, its time derivative and kinetic temperature gradient showed that the characteristic relaxation times of the nonequilibrium flux within the nonlocal Cattaneo model at temperatures $10\,\mathrm{K} < T < 40\,\mathrm{K}$ are very small ($\tau_v < 10^{-11}$ s) and, comparable with the time of phonons free path.

Introduction

The nonequilibrium heat transfer process is described in the conventional approach accepted in the continuum mechanics by means of parabolic type heat equation with inherent paradox of infinite propagation velocity. This fact indicates that this model has limits in its application, and it makes it interesting to investigate the conditions when the local thermodynamic equilibrium and locality principles are used for the description of non-stationary heat transfer based on the Fourier law

$$\vec{q}(\vec{x},t) = -\lambda(T)\nabla T(\vec{x},t). \tag{1}$$

becomes unsuitable. Here $T(\vec{x},t)$ is the temperature, $\vec{q}(\vec{x},t)$ – heat flux, $\lambda(T)$ – thermal conductivity.

One type of non-local heat and mass transfer models is based on the Cattaneo approach [1,2]. In this model the heat flux relaxation time τ_v is introduced. Based on this modification the equilibrium and generalized Fourier's law are written as

$$\vec{q}(\vec{x},t) + \tau_v \frac{\partial q(\vec{x},t)}{\partial t} = -\lambda(T)\nabla T(\vec{x},t). \tag{2}$$

and the traditional equation of thermal conductivity of parabolic type is converted to a telegraph equation of the hyperbolic type [3] with a limited speed (V_τ) of the disturbances propagation

$$V_\tau = \sqrt{\frac{\chi}{\tau_v}}. \tag{3}$$

Here $\chi = \lambda/\rho C_V$ – thermal diffusivity, ρ – density, C_V – thermal capacity.

The heat transfer process was numerically simulated in [3], by means of molecular dynamics (MD) method for the three-dimensional (3D) Lennard–Jones (LJ) system having small number of particles (512), where the thermal conductivity was calculated as

$$\lambda = \frac{\Omega}{3k_B T^2}\int_0^\infty \langle q_l(0)q_l(t)\rangle dt, \tag{4}$$

$$\langle q_l(0)q_l(t)\rangle = \langle q_l(0)q_l(0)\rangle \exp(-t/\tau_v). \tag{5}$$

Here Ω – volume, $q_l - q_l$ – l-component of heat flux, τ_v defines the parameter of the Cattaneo model and it was calculated as

$$\tau_v = \frac{\lambda k_B T^2}{\langle q_l(0)q_l(0)\rangle \Omega}. \tag{6}$$

Phonon relaxation time for the system considered was equal to

$$\tau_{ph} = 3\lambda/\rho C_V c_s^2 \tag{7}$$

and had the order 10^{-11} s for temperature interval $60\,\mathrm{K} < T < 130\,\mathrm{K}$. Here c_s – sound velocity.

MD methods are widely used for modeling of thermal processes in the microsystems. Typically the LJ potential is used to describe

* Corresponding author.

http://dx.doi.org/10.1016/j.rinp.2016.05.003
2211-3797/